

Benzthiazuron, HFBA

Inchi:	InChI=1S/C14H10F7N3O2S/c1-23(9(25)12(15,16)13(17,18)14(19,20)21)11(26)24(2)10-2
InchiKey:	VOHGAKJNHUAGHA-UHFFFAOYSA-N
Formula:	C14H10F7N3O2S
SMILES:	CN(C(=O)N(C)c1nc2ccccc2s1)C(=O)C(F)(F)C(F)(F)C(F)(F)F
Mol. weight [g/mol]:	417.30

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.19		Crippen Method
logp	4.144		Crippen Method
mcvol	231.020	ml/mol	McGowan Method
rinpola	1959.00		NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R220205&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpola:	Non-polar retention indices

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<https://www.chemeo.com/cid/15-982-5/Benzthiazuron-HFBA.pdf>

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